CLUSTER EXPANSIONS IN MANY-FERMION THEORY

I. "FACTOR-CLUSTER" FORMALISMS*

by

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ABSTRACT

Cluster development may furnish a powerful device for the calculation of the expectation values of the observables of a many-fermion system with respect to dynamically correlated state vectors. The generalized normalization integral, a generating function for the required expectation values, is defined, and four of the many possible decompositions of this function into cluster integrals are explored. Two of these decompositions are slight extensions of the conventional ones of Iwamoto and Yamada and Aviles, Hartogh, and Tolhoek. The other two are product decompositions, leading to new, "factor-cluster" formalisms. A factor-cluster expansion is applied to the evaluation of the η-particle spatial distribution function.

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1. Introduction

In this paper we shall explore the formal aspects of cluster expansions as a tool for the systematic evaluation of expectation values of the observables of a system of N identical fermions with respect to dynamically correlated state vectors. The techniques to be developed may be useful in the calculation of properties of the bound states of such finite systems as nuclei and the electronic subsystems of atoms and molecules in the fixed nuclei approximation, and of such infinite systems as quantum fluids (including liquid He^3 and nuclear matter) and quantum solids (solid He^3).

In treating a many-fermion system one usually starts with some intelligently chosen independent-particle model and then corrects this model for its most disconcerting inadequacies. There will in general be important correlation effects, whose description is by definition outside the scope of the input independent-particle model. We shall devote the major portion of this introduction to a discussion of how correlation effects may be built into the assumed form for the many particle wave function.

The correlation structure of the exact stationary state wave function has been investigated by many authors.[1-11] Their discoveries may be conveniently reviewed in terms of the highly formal expression

$$\Psi_{\underset{\sim}{m}}(x_1 \cdots x_N) = \frac{1}{\sqrt{N!}} \langle 0 | \psi(x_N) \cdots \psi(x_1) \, \mathcal{T}_{\underset{\sim}{m}} \, a^+_{m_N} \cdots a^+_{m_1} | 0 \rangle \qquad (1)$$

for the exact wave function. Here a_κ^+ and a_κ are the usual fermion creation and annihilation operators associated with a complete set of single-particle states. The one-particle field operator $\psi(x_i)$ is a linear combination

$$\psi(x_i) = \sum_\kappa \varphi_\kappa(x_i)\, a_\kappa \qquad (2)$$

of the annihilation operators a_κ, the coefficients $\varphi_\kappa(x_i)$ being the configuration-space representatives of the single-particle states κ. The argument x_i stands for all the coordinates - space ($\underset{\sim}{r}_i$), spin (s_{z_i}), and, when appropriate, isospin (t_{z_i}) - of the i th particle. $|0\rangle$ is the zero-particle state, the vacuum. The specific ket $|\Phi_{\underset{\sim}{m}}\rangle = a_{m_N}^+ \cdots a_{m_1}^+ |0\rangle$, a (N-particle) basis ket of the occupation number representation generated by the a_κ^+'s represents the (input) independent-particle approximation to the exact N-fermion state of interest. We use $\underset{\sim}{m}$ to denote the collection of labels $m_1, m_2, \cdots, m_N$, and, to be definite, take $m_1 < m_2 < \cdots < m_N$. The basis $\{|\varphi_\kappa\rangle\}$ of single-particle kets, or orbitals, may, for example, be chosen according to the Hartree-Fock scheme, the $N \times N$ determinant of a particular set of N such orbitals yielding a "self-consistent solution" to the N-body problem. The ket $|\Psi_{\underset{\sim}{m}}\rangle$ corresponding to the wave function $\Psi_{\underset{\sim}{m}}(x_1 \cdots x_N)$ as given in (1) is supposed to have unit overlap with $|\Phi_{\underset{\sim}{m}}\rangle$. $\mathcal{F}_{\underset{\sim}{m}}$, <u>the correlation operator</u>, serves to convert

$$\gamma^{\underset{\sim}{m}}_{m_{j(1)}} = \beta^{\underset{\sim}{m}}_{m_{j(1)}}$$

$$\gamma^{\underset{\sim}{m}}_{m_{j(1)} m_{j(2)}} = \beta^{\underset{\sim}{m}}_{m_{j(1)}} \beta^{\underset{\sim}{m}}_{m_{j(2)}} + \beta^{\underset{\sim}{m}}_{m_{j(1)} m_{j(2)}}$$

$$\vdots \qquad (8)$$

$$\gamma^{\underset{\sim}{m}}_{m_{j(1)} \cdots m_{j(n)}} = \sum_{k=1}^{n} \left\{ \sum_{\substack{\text{all partitions} \\ \text{of } m_{j(1)} \cdots m_{j(n)} \\ \text{among } n-k+1 \ \beta\text{'s}}} \beta^{\underset{\sim}{m}}_{\cdots} \beta^{\underset{\sim}{m}}_{\cdots} \cdots \beta^{\underset{\sim}{m}}_{\cdots} \right\}$$

of the excitation operators γ in terms of the <u>irreducible cluster operators</u> β, and invoking the (essentially obvious) facts that any two β...'s commute and the product of two β...'s with overlapping indices is zero, $\mathcal{F}_{\underset{\sim}{m}}$ may readily be cast into the product form

$$\mathcal{F}_{\underset{\sim}{m}} = \left\{ \prod_{i=1}^{N} (1 + \beta^{\underset{\sim}{m}}_{m_i}) \right\} \left\{ \prod_{i<j} (1 + \beta^{\underset{\sim}{m}}_{m_i m_j}) \right\} \left\{ \prod_{i<j<k} (1 + \beta^{\underset{\sim}{m}}_{m_i m_j m_k}) \right\}$$

$$\cdots \left\{ 1 + \beta^{\underset{\sim}{m}}_{m_1 \cdots m_N} \right\} . \qquad (9)$$

As opposed to the aforementioned expansions for $\Psi_{\underset{\sim}{m}}$, (1) with (9) inserted displays a very clean separation of one-body, two-body, . . . n-body, ... correlation effects. A single correlation factor operator $1 + \beta^{\underset{\sim}{m}}_{m_{j(1)} \cdots m_{j(n)}}$ appears for each of the $N!/[(N-n)!\,n!]$ distinct

clustering possibilities for particles in n orbitals selected from the set $\varphi_{m_1} \cdots \varphi_{m_N}$, there being $2^N - 1$ factors in all. Now, if we want an approximation for $\Psi_{\underset{\sim}{m}}$ which includes all correlation effects involving groups of, say, n or less particles, we simply put all $\beta^{\underset{\sim}{m}}_{m_{l(1)} \cdots m_{l(p)}}$'s with $p > n$ equal to zero.

It is interesting to note that a cluster decomposition law plays an important role even at this most elemental stage in the development of a many-body theory.

These formal manipulations, however, bring us no closer to a solution of the many-body problem since the c's, the basic ingredients of the γ's (or U's) and therefore the basic ingredients of the β's, still remain to be determined, for example by a perturbative or variational calculation. Obviously, direct determination of the β's would be highly desirable.[2,3,4]

Another form of correlated wave function that we shall consider is a generalization of the Jastrow wave function:[12,13]

$$\tilde{\Psi}_{\underset{\sim}{m}}(x_1 \cdots x_N) = \mathcal{A}(N) \left[F_{\underset{\sim}{m}}(x_1 \cdots x_N)\, \varphi_{m_1}(x_1) \cdots \varphi_{m_N}(x_N) \right], \qquad (10)$$

where

$$F_{\underset{\sim}{m}}(x_1 \cdots x_N) = \prod_{n=1}^{N} \prod_{\langle j(1) \cdots j(n) | 1 \cdots N \rangle} f^{\underset{\sim}{m}}_{m_{j(1)} \cdots m_{j(n)}}(x_{j(1)} \cdots x_{j(n)}). \qquad (11)$$

We adopt here and henceforth the notation $\langle j(1) \cdots j(k) | l(1) \cdots l(p) \rangle$, $k \leq p$, for a particular combination of k indices, these

selected from the set of indices $\{l_{(1)} \cdots l_{(p)}\}$. The special case $\langle j_{(1)} \cdots j_{(k)} | 1 \cdots N \rangle$ will be abbreviated to $\langle j_{(1)} \cdots j_{(k)} \rangle$. In (11) the correlation function $f^{m}_{m_{j(1)} \cdots m_{j(n)}}(x_{j(1)} \cdots x_{j(n)})$ - which one might hope to determine variationally - describes correlations of n particles which, in the independent-particle approximation, occupy single-particle states $m_{j(1)} \cdots m_{j(n)}$. (Observe that in the primitive function, i.e., the bracketed expression in (10), a 1-1 correspondence exists between the orbital and particle labels; application of the antisymmetrizer eradicates this correspondence and restores the indistinguishability of the particles.) If we choose all $N!/[(N-n)!\,n!]$ of the n-particle correlation functions to be the same symmetric function of their n coordinate arguments, (10)-(11) simplifies to

$$\tilde{\Psi}_{\underset{\sim}{m}}(x_1 \cdots x_N) = F_{\underset{\sim}{m}}\, \Phi_{\underset{\sim}{m}}(x_1 \cdots x_N) , \tag{12}$$

where

$$\Phi_{\underset{\sim}{m}}(x_1 \cdots x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{m_1}(x_1) & \cdots & \varphi_{m_N}(x_1) \\ \vdots & & \vdots \\ \varphi_{m_1}(x_N) & \cdots & \varphi_{m_N}(x_N) \end{vmatrix} \tag{13}$$

and

$$F_{\underset{\sim}{m}} = \prod_{n=1}^{N} \prod_{\langle j(1) \cdots j(n) \rangle} f^{m}_{n}(x_{j(1)} \cdots x_{j(n)}) . \tag{14}$$

Upon setting $f^{\underset{\sim}{m}}_{n} = 1$, $n \neq 2$, (12) - (14) collapses to the definition of the well-known Jastrow wave function.

The product form (10) bears a superficial resemblance to the exact stationary state wave function written in terms of the product form for $\mathcal{F}_{\underset{\sim}{m}}$. However, it is really of quite different character, since, unlike $\prod_{\langle j(1)\cdots j(n)\rangle}(1+\beta^{\underset{\sim}{m}}_{m_{j(1)}\cdots m_{j(n)}})$, which produces only the effects of all specifically n-body correlations, $\prod_{\langle j(1)\cdots j(n)\rangle} f^{\underset{\sim}{m}}_{m_{j(1)}\cdots m_{j(n)}}$ incorporates not only irreducible n-body correlation effects but also correlation effects involving all larger groups of particles, these being incorporated in terms of <u>products</u> of n-body correlation functions. Thus, as in those cases of the expansion arising when (3) is inserted into (1) and the expansion (5) of Sinanoğlu, there is, in (10) or (12), no clean separation of correlation effects, but the mixing, in these latter forms for the wave function, is not intrinsically of such a nature as to vitiate their use in practical calculations and may even be beneficial.

Since we are thinking in terms of stationary states, we may regard $\Psi_{\underset{\sim}{m}}$ of (1)-(3) or (5)-(7) as the exact wave function for our problem (or, with undetermined c's, as a trial wave function) and $\tilde{\Psi}_{\underset{\sim}{m}}$ of (10)-(11), (12)-(14) as trial wave functions.

We remind the reader that any of the above wave functions may alternatively be viewed as the element $\underset{\sim}{m}$ of a <u>basis of correlated functions</u> which, depending on how the $f^{\underset{\sim}{m}}_{m_{j(1)}\cdots m_{j(k)}}$'s $f^{\underset{\sim}{m}}_{k}$'s or $c_{\cdots}$'s are chosen, may provide a highly advantageous starting point for exact description of the N-fermion system, a

far more appropriate starting point then the input independent-particle basis.[13,14,15]

Now let us turn to the task at hand. Working henceforth entirely in the configuration space representation, our attention is centered on integrals like

$$(\Psi, S\Psi) \equiv \int \prod_{b=1}^{N} dx_b \, \Psi^*(x_1 \cdots x_N) \, S(1 \cdots N) \, \Psi(x_1 \cdots x_N) \qquad (15)$$

and

$$(\Psi, \Psi) \equiv \int \prod_{b=1}^{N} dx_b \, |\Psi(x_1 \cdots x_N)|^2 \, , \qquad (16)$$

where $S(1 \cdots N)$ is a permutation-symmetric Hermitian operator and $\int \prod_{b=1}^{N} dx_b$ implies integrations over all continuous coordinates and summations over all discrete ones. (When written as an argument of an operator, i stands for $\underset{\sim}{r}_i$, $-i\hbar \underset{\sim}{\nabla}_i$, and the spin and (if appropriate) isospin operators $\underset{\sim}{\sigma}_i$, $\underset{\sim}{\tau}_i$.) The methods to be developed for the evaluation of the ratio (15)/(16), the expectation value

$$\langle S \rangle = \frac{(\Psi, S\Psi)}{(\Psi, \Psi)} \, , \qquad (17)$$

are sufficiently general that Ψ may be any of the forms we have considered, in fact, any N-particle wave function. We have dropped

the $\underset{\sim}{m}$ label, since we shall deal from now on with a particular state. (This allows a welcome simplification of the notation as regards single-particle state labels - we shall be able to write $j(1) \cdots j(n)$ in place of $m_{j(1)} \cdots m_{j(n)}$.)

In the absence of dynamical correlations (all β's except possibly the one-particle ones set zero, giving an independent-particle approximation) the evaluation of (17) is usually trivial. For example, if we take S to be the ordinary Hamiltonian, a symmetric sum of one-body operators plus a symmetric sum of two-body operators, the required expectation value reduces quickly to a sum of one-body integrals plus a sum of two-body integrals. But in general it is a practical impossibility to conclude the operations indicated in (17). Thus one is prompted to express (17) as a sum of one-body terms, plus a sum of two-body terms, ..., plus a sum of N-body terms, in such way that truncation of the series after a manageable number of terms involving only calculable (few-body) integrals, furnishes (hopefully) a useful approximation. Expansions of this type, called cluster expansions, first saw application in the classical statistical mechanics of imperfect gases, where they have long been employed to approximate the partition function.[16] Two cluster expansions, the one associated with Iwamoto and Yamada[17] (IY) and the other with Aviles[18] and Hartogh and Tolhoek[19] (AHT), have frequently been used in quantum mechanical many-body calculations. In Section 2 the generalized normalization integral - a quantity from which the required expectation values may be extracted - is

defined, and decomposed into cluster integrals according to schemes closely allied with those of IY and AHT. Then two radically different ("factor-cluster") decompositions, bearing the same relation to the Van Kampen[20] classical cluster development as that borne by the IY and AHT decompositions to the classical Ursell[16] development, are studied in detail. To conclude Section 2, general formulae for the expectation value of an operator in terms of the two new sets of cluster integrals are derived. An application of these formulae to the evaluation of the n-particle spatial distribution function is presented in Section 3. The final section is devoted to a general comparison of the four formalisms here studied, in the context of their practical application for the systems of interest.

In the second paper of this series we shift the emphasis from an investigation of the new factor-cluster formalisms per se to an exploitation of their properties and their relationships with the IY and AHT formalisms, with the aim of extending the applicability of these latter formalisms to finite N .

2. The Cluster Expansions

A symmetric Hermitian operator $S(1\ldots N)$ may in general be resolved into a symmetric sum of one-body operators, plus a symmetric sum of two-body operators, ... plus a symmetric sum of N-body operators:

$$S(1\ldots N) = \sum_{i=1}^{N} S_i(1\ldots N) \qquad (18)$$

with

$$S_p(1\ldots N) = \sum'_{\langle j(1)\cdots j(p)\rangle} \bar{S}_p(j(1)\cdots j(p)), \tag{19}$$

where $\bar{S}_p(j(1)\cdots j(p))$ operates in the subspace of the particles labeled $j(1)\cdots j(p)$. There are in general many possible ways of resolving $S(1\ldots N)$. There will always be one particular resolution in which none of the $\bar{S}_p(j(1)\cdots j(p))$ may be further decomposed into the sum of terms which individually depend on a proper subset of particle labels $j(1),\ldots,j(p)$. Such a resolution will be said to be irreducible.

For example, the Hamiltonian of a system of N identical, non-relativistic particles of mass M, located in an external field $V(i)$ and interacting via two-body potentials $v(i,j)$,

$$H(1\ldots N) = \sum_{i=1}^{N} \frac{-\hbar^2}{2M}\nabla_i^2 + \sum_{i=1}^{N} V(i) + \sum'_{1\le i<j\le N} v(i,j), \tag{20}$$

may, as suggested above, be irreducibly resolved by taking

$$\begin{aligned} \bar{S}_1(i) &= \frac{-\hbar^2}{2M}\nabla_i^2 + V(i), \\ \bar{S}_2(i,j) &= v(i,j), \\ \bar{S}_n(j(1)\cdots j(n)) &= 0, \qquad 3 \le n \le N. \end{aligned} \tag{21}$$

As a second illustration, consider the operator

$$P^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n ; \underset{\sim}{r}_1' \cdots \underset{\sim}{r}_N') = \sum_{\langle j(1) \cdots j(n) \rangle} \left\{ \sum_{\substack{\text{all permutations} \\ \text{of } \ell(1) \cdots \ell(n) \\ \text{over } 1 \cdots n}} \prod_{i=1}^{n} \delta(\underset{\sim}{r}_{\ell(i)} - \underset{\sim}{r}_{j(i)}') \right\} \quad (22)$$

whose expectation value yields the n-particle spatial distribution function

$$\rho^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n) = \frac{N!}{(N-n)!} \times \frac{\sum_{\substack{\text{all spin} \\ \text{coordinates}}} \int \prod_{i=n+1}^{N} d\underset{\sim}{r}_i \, \Psi^*(x_1' \cdots x_N') \Psi(x_1 \cdots x_N)}{\int \prod_{i=1}^{N} dx_i \, \Psi^*(x_1' \cdots x_N') \Psi(x_1 \cdots x_N)} \quad (23)$$

In this case the obvious choice of $\bar{S}_\rho$'s is

$$\bar{S}_n^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n ; \underset{\sim}{r}_{j(1)}' \cdots \underset{\sim}{r}_{j(n)}') = \left\{ \sum_{\substack{\text{all permuta-} \\ \text{tions of} \\ \ell(1) \cdots \ell(n) \text{ over} \\ 1 \cdots n}} \prod_{i=1}^{n} \delta(\underset{\sim}{r}_{\ell(i)} - \underset{\sim}{r}_{j(i)}') \right\},$$

$$\bar{S}_\rho^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n ; \underset{\sim}{r}_{j(1)}' \cdots \underset{\sim}{r}_{j(\rho)}') = 0, \quad \rho \neq n. \quad (24)$$

Again the resolution we have chosen is irreducible.

Following the lead of Iwamoto and Yamada[17] we define the (generalized) normalization integral

$$I_{\underset{\sim}{m}}(\alpha) = \int \prod_{b=1}^{N} dx_b \, \Psi^{*}_{\underset{\sim}{m}}(x_1 \cdots x_N) \, e^{\alpha S(1\cdots N)} \, \Psi_{\underset{\sim}{m}}(x_1 \cdots x_N)$$

$$= \int \prod_{b=1}^{N} dx_b \, \Psi^{*}_{\underset{\sim}{m}} \left[1 + \alpha S + \frac{\alpha^2}{2!} S^2 + \cdots \right] \Psi_{\underset{\sim}{m}} \tag{25}$$

from which the required expectation value may be obtained by means of the following differentiation:

$$\langle S \rangle = \left. \frac{\frac{d}{d\alpha} I_{\underset{\sim}{m}}(\alpha)}{I_{\underset{\sim}{m}}(\alpha)} \right|_{\alpha=0} = \left. \frac{d}{d\alpha} \ln I_{\underset{\sim}{m}}(\alpha) \right|_{\alpha=0} . \tag{26}$$

Our goal is to calculate $I_{\underset{\sim}{m}}(\alpha)$ or, alternatively, $\ln I_{\underset{\sim}{m}}(\alpha)$ by the technique of cluster expansion. Although we are presently interested only in the expectation value of the operator $S_{(1\cdots N)}$, it might be pointed out that a knowledge of $I_{\underset{\sim}{m}}(\alpha)$ yields a wealth of additional information. In particular, the variance of $S_{(1\cdots N)}$ may be computed as the second derivative of $\ln I_{\underset{\sim}{m}}(\alpha)$ evaluated at $\alpha = 0$.[21] Finally, let us note that the basic idea embodied in (25) and (26) has recently been extended by Clark and Westhaus[13] to the evaluation of non-diagonal matrix elements in the representation defined by a set of dynamically correlated basis functions.

Our procedures for calculating $I_{\underset{\sim}{m}}(\alpha)$ begin with the recognition that, given $\Psi_{\underset{\sim}{m}}$ and $S_{(1\cdots N)}$, a set of related functions and operators may be defined for n-particle subspaces,

$n \leq N$, of the N-particle Hilbert space. First, we consider a subset $m_{j(1)} \cdots m_{j(n)}$ of $\underset{\sim}{m}$ and construct an n-particle "wave-function". In particular, according as form (1) with (3) inserted, form (5), form (10), or form (12) has been chosen for $\Psi_{\underset{\sim}{m}}$, we define the n-particle "wave function" respectively, as

$$\Psi^{(x_{j(1)} \cdots x_{j(n)})}_{m_{j(1)} \cdots m_{j(n)}} = \frac{1}{\sqrt{n!}} \langle 0 | \Psi_{(x_{j(n)})} \cdots \Psi_{(x_{j(1)})} \left\{ \prod_{p=1}^{n} (1 + \beta_{m_{j(p)}}) \right\} \cdot$$

$$\left\{ \prod_{p<q}^{n} (1 + \beta_{m_{j(p)} m_{j(q)}}) \right\} \cdots \left\{ 1 + \beta_{m_{j(1)} \cdots m_{j(n)}} \right\} a^{\dagger}_{m_{j(n)}} \cdots a^{\dagger}_{m_{j(1)}} | 0 \rangle , \tag{27a}$$

$$\Psi^{(x_{j(1)} \cdots x_{j(n)})}_{m_{j(1)} \cdots m_{j(n)}} = Q(n) \left[\prod_{i=1}^{n} \varphi^{(x_{j(i)})}_{m_{j(i)}} + \sum_{p=1}^{n} \prod_{i \neq p}^{n} \varphi^{(x_{j(i)})}_{m_{j(i)}} U^{\underset{\sim}{m}}_{(x_{j(p)}) m_{j(p)}} + \right.$$

$$\left. + \frac{1}{2!} \sum_{p<q}^{n} \prod_{i \neq p,q}^{n} \varphi^{(x_{j(i)})}_{m_{j(i)}} U^{\underset{\sim}{m}}_{(x_{j(p)} x_{j(q)}) m_{j(p)} m_{j(q)}} + \cdots \frac{1}{\sqrt{n!}} U^{\underset{\sim}{m}}_{(x_{j(1)} \cdots x_{j(n)}) m_{j(1)} \cdots m_{j(n)}} \right] , \tag{27b}$$

$$\Psi^{(x_{j(1)} \cdots x_{j(n)})}_{m_{j(1)} \cdots m_{j(n)}} = Q(n) \left[\prod_{p=1}^{n} \left\{ \frac{\prod f^{\underset{\sim}{m}}_{m_{\ell(1)} \cdots m_{\ell(p)}} (x_{\ell(1)} \cdots x_{\ell(p)})}{\langle \ell(1) \cdots \ell(p) | j(1) \cdots j(n) \rangle} \right\} \prod_{q=1}^{n} \varphi^{(x_{j(q)})}_{m_{j(q)}} \right] , \tag{27c}$$

or

$$\Psi^{(x_{j(1)} \cdots x_{j(n)})}_{m_{j(1)} \cdots m_{j(n)}} = \prod_{p=1}^{n} \left\{ \frac{\prod f^{\underset{\sim}{m}}_{p} (x_{\ell(1)} \cdots x_{\ell(p)})}{\langle \ell(1) \cdots \ell(p) | j(1) \cdots j(n) \rangle} \right\} \cdot \frac{1}{\sqrt{n!}} \begin{vmatrix} \varphi^{(x_{j(1)})}_{m_{j(1)}} & \cdots & \varphi^{(x_{j(n)})}_{m_{j(n)}} \\ \vdots & & \vdots \\ \varphi^{(x_{j(n)})}_{m_{j(1)}} & \cdots & \varphi^{(x_{j(n)})}_{m_{j(n)}} \end{vmatrix} . \tag{27d}$$

In the second and third definitions $Q(n)$ is the antisymmetrizer for the appropriate set of n coordinate labels, normalized such that $(Q(n))^2 = \sqrt{n!}\, Q(n)$. Although we have written the $\Psi_{m_{j(1)} \cdots m_{j(n)}}$ as functions of the coordinates $x_{j(1)}, \cdots, x_{j(n)}$, they can, of course, be written in terms of any set of n coordinates - i.e., there is no necessary correspondence between the place indices of the selected orbitals $m_{j(1)}, m_{j(2)}, \cdots, m_{j(n)}$ and the coordinate labels (see Eq. (29)). Henceforth, the orbital indices $m_{j(1)}, \cdots, m_{j(n)}$ will, for brevity, be written simply as $j(1) \cdots j(n)$; moreover, the same symbol $\Psi_{j(1) \cdots j(n)}$ will denote, as appropriate, any of the four forms of the n-particle "wave function". Next, from the elements into which $S(1 \cdots N)$ is resolved via (18) and (19), we construct the n-particle operator

$$S(1 \cdots n) = \sum_{p=1}^{n} \sum_{\langle \ell(1) \cdots \ell(p) | 1 \cdots n \rangle} \bar{S}_p(\ell(1) \cdots \ell(p)) \,. \tag{28}$$

Then we define, in terms of a particular n-particle wave function and n-particle operator a subnormalization integral indexed with

the same orbital labels as designate the corresponding n-particle wave function:

$$I^{(\alpha)}_{j(1)\cdots j(n)} = \int \prod_{b=1}^{n} dx_b \, \Psi^{*}_{(x_1 \cdots x_n)\, j(1)\cdots j(n)} \, e^{\alpha S(1\cdots n)} \, \Psi_{(x_1 \cdots x_n)\, j(1)\cdots j(n)} \,. \tag{29}$$

Counting $I^{(\alpha)}_{1\cdots N} = I_{\underset{\sim}{m}}(\alpha) \equiv I(\alpha)$ as a particular subnormalization integral, we see there are $2^N - 1$ such quantities, each indexed by a particular subset of orbital labels, $j(1), \ldots, j(n)$.

Before proceeding to general techniques for the evaluation of $I(\alpha)$ let us imagine for a moment that all correlations among the particles have ceased to exist (e.g. all β operators vanish) and that all except the one-body terms in the operator $S(1\cdots n)$ are zero. Under these conditions we have

$$I^{(\alpha)}_{j(1)\cdots j(n)} \longrightarrow \tilde{I}^{(\alpha)}_{j(1)\cdots j(n)} = \frac{1}{n!} \int \prod_{b=1}^{n} dx_b \left| \begin{matrix} \varphi_{j(1)}(x_1) & \cdots & \varphi_{j(n)}(x_1) \\ \vdots & & \vdots \\ \varphi_{j(1)}(x_n) & \cdots & \varphi_{j(n)}(x_n) \end{matrix} \right|^{*} e^{\alpha \sum_{i=1}^{n} \bar{S}_1(i)} \left| \begin{matrix} \varphi_{j(1)}(x_1) & \cdots & \varphi_{j(n)}(x_1) \\ \vdots & & \vdots \\ \varphi_{j(1)}(x_n) & \cdots & \varphi_{j(n)}(x_n) \end{matrix} \right|$$

$$= \prod_{i=1}^{n} \left[\int dx_1 \varphi^{*}_{j(i)}(x_1) \, e^{\alpha \bar{S}_1(1)} \, \varphi_{j(i)}(x_1) \right] + O(\alpha^2)$$

$$= \prod_{i=1}^{n} \tilde{I}^{(\alpha)}_{j(i)} + O(\alpha^2) \,. \tag{30}$$

In particular, if the operator $\bar{S}_1(1) = h_0(1)$ is a one-body Hamiltonian containing some ad hoc single-particle potential and $\{\varphi_1, \varphi_2, \cdots, \varphi_N\}$ a set of eigenfunctions of h_0, then the equalities in (30) hold with the addends $O(\alpha^2)$ omitted. Frequently, such an independent-particle model provides both a convenient image of the physical system and a framework in which those observables corresponding to single-particle operators may be accurately calculated. In any event, as long as we are only interested in computing $\langle S \rangle$ terms $O(\alpha^2)$ need never be considered.

We are now prepared to set forth the essential structure and state the underlying philosophy of a wide class of cluster formalisms applicable to the evaluation of $I(\alpha)$. Each of the above subnormalization integrals $I_{j(1)\cdots j(n)}$ or, more generally, some linear combination of those with the given number n of indices, is to be built up from the $\tilde{I}_{j(i)}$'s and a (finite) number of cluster integrals involving anywhere from one- to n-fold integrations. Alternatively, we say that the subnormalization integral, or the corresponding linear combination of subnormalization integrals, is decomposed into the $\tilde{I}_{j(i)}$'s and the cluster integrals. With the $\tilde{I}_{j(i)}$'s and the $I_{j(1)\cdots j(n)}$'s already defined by (30) and (29) respectively, such a decomposition equation provides the definition of the last appearing, n-body, cluster integral. Proceeding to $n = N$, an expansion for $I(\alpha)$ in terms of the cluster integrals is achieved. We shall see that for some decompositions (among these the most familiar) it is necessary to rearrange this primitive cluster expansion for $I(\alpha)$ in order to

obtain a useful approximation scheme for large N . All of the primitive cluster expansions to be considered will contain a finite number of addends for finite N .

Different modes of decomposition of the basic subnormalization integrals, or appropriate linear combinations of them, lead to different definitions of the cluster integrals. But an important feature of general cluster theory as herein circumscribed will pervade all the following considerations for finite N : no matter what mode of decomposition is chosen, the explicit elimination of all the cluster integrals from the decomposition equation for, say, $I_{j(1)\cdots j(n)}$ must lead to an identity. In particular, it is the definition of the last cluster integral which ensures that the (primitive) cluster expansion for $I_{(\alpha)}$, if completely summed, will regenerate this normalization integral. This feature is trivially obvious, but, as we shall see, formally useful.

Later discussions will be facilitated if we adopt a definite convention for what we shall mean by a term contributing to a cluster expansion of some quantity. Any individual contribution to a given cluster expansion will always be a product of the corresponding cluster integrals (perhaps with only one such factor), supplemented by some numerical factor. These cluster integrals may or may not be indexed with single-particle labels. In the former case, the term corresponding to the contribution in question will consist of this contribution, summed over all combinations of the allowed single-particle labels, the original labels having been replaced by dummies.

In the latter case, the term corresponding to the contribution is that contribution multiplied by the number of times it occurs in the expansion. In both cases, if the contribution enters with a minus sign, that also is to be attached. The given cluster expansion is, of course, the sum of all such unique terms. The meaning of this convention will become clearer as we develop concrete examples of cluster expansions.

In the above we have not specified any essential properties that the cluster integrals must possess, but have merely regarded them as the elements of the postulated decomposition - which of course determines their properties completely. It is not our immediate concern whether or not a given n-body cluster integral (involving integrations over n sets x_b) so determined is irreducible in the sense that this integral can be in turn decomposed into a sum of products of independent integrals over fewer than n sets of coordinates. Of course, a careful study of the structure of the cluster integrals, in particular with respect to their possible reducibility, is vital in analyzing the behavior of the terms in a cluster expansion as N grows large.[13,14,22,23]

To conclude these very general remarks: Although, strictly speaking, every cluster expansion is a tautology, the value of a given cluster formalism, when employed in its main role of generating approximations for $\langle S \rangle$, depends on the wisdom of our decomposition. We shall always have in mind systems for which irreducible correlations involving many particles are less important than those involving few.

Thus we always seek a cluster expansion for $\langle S \rangle$ which, perhaps after suitable rearrangement, will reflect this situation in rapid convergence, allowing us to approximate $\langle S \rangle$ satisfactorily in terms of the first few cluster integrals, therefore in terms of the first few subnormalization integrals. Naturally, the usefulness of a given cluster expansion of the expectation value of the observable S will depend crucially on the correlated wave function chosen; in the final analysis the merit of the approximation schemes suggested by this paper must be tested by detailed numerical calculations.

We shall now study in detail four modes of defining cluster integrals. The first is a straightforward extension of the procedure adopted by Iwamoto and Yamada.[17] Initially we approximate $I^{(\alpha)}_{j(1)\cdots j(n)}$ by the product $\prod_{i=1}^{n} \tilde{I}^{(\alpha)}_{j(i)}$ and then "build up" the subnormalization integral by replacing each combination of zero, one, two, ... n factors in $\prod_{i=1}^{n} \tilde{I}^{(\alpha)}_{j(i)}$ with the sum of all possible products of one-body, two-body, ... n-body cluster integrals involving, with no repetitions, the same set of indices as the replaced factors. Beginning with the one-indexed quantities, a hierarchy of equations is generated:

$$
\begin{aligned}
I_{j(1)} &= \tilde{I}_{j(1)} + X_{j(1)} \,, \\
I_{j(1)j(2)} &= \tilde{I}_{j(1)}\tilde{I}_{j(2)} + X_{j(1)}\tilde{I}_{j(2)} + \tilde{I}_{j(1)}X_{j(2)} + X_{j(1)}X_{j(2)} + X_{j(1)j(2)} \,, \\
I_{j(1)j(2)j(3)} &= \prod_{i=1}^{3} \tilde{I}_{j(i)} + \sum_{i=1}^{3}\left[X_{j(i)}\prod_{\substack{p=1\\ p\neq i}}^{3}\tilde{I}_{j(p)} + \tilde{I}_{j(i)}\prod_{\substack{p=1\\ p\neq i}}^{3}X_{j(p)}\right] + \\
&\qquad \sum_{i=1}^{3}\left(\sum_{\substack{p<q\\ p,q\neq i}}\left[\tilde{I}_{j(i)} + X_{j(i)}\right]X_{j(p)j(q)}\right) + \prod_{i=1}^{3}X_{j(i)} + X_{j(1)j(2)j(3)} \\
&\quad \vdots \\
I_{12\cdots N} &= \prod_{i=1}^{N}\tilde{I}_i + \sum_{i=1}^{N}X_i\prod_{p\neq i}\tilde{I}_p + \cdots X_{12\cdots N} \,.
\end{aligned}
\tag{31}
$$

Introducing the normalized cluster integrals

$$X_{j(1)\cdots j(n)} = \frac{\Sigma_{j(1)\cdots j(n)}}{\prod_{i=1}^{n} \tilde{I}_{j(i)}} \tag{32}$$

we can rewrite these decomposition equations as

$$I_{j(1)} = \tilde{I}_{j(1)} \cdot [1 + X_{j(1)}],$$

$$I_{j(1)j(2)} = \tilde{I}_{j(1)} \tilde{I}_{j(2)} [1 + X_{j(1)} + X_{j(2)} + X_{j(1)} X_{j(2)} + X_{j(1)j(2)}];$$

$$I_{j(1)j(2)j(3)} = \prod_{i=1}^{3} \tilde{I}_{j(i)} \Big[1 + \sum_{p=1}^{3} X_{j(p)} + \sum_{1 \le p < q \le 3} (X_{j(p)} X_{j(q)} + X_{j(p)j(q)}) +$$

$$X_{j(1)} X_{j(2)} X_{j(3)} + X_{j(1)} X_{j(2)j(3)} + X_{j(2)} X_{j(1)j(3)} +$$

$$X_{j(3)} X_{j(1)j(2)} + X_{j(1)j(2)j(3)}\Big], \tag{33}$$

$$\vdots$$

$$I_{12\cdots N} = I = \prod_{i=1}^{N} \tilde{I}_i \Big[1 + \sum_{p} X_p + \sum_{p<q} (X_p X_q + X_{pq}) + \cdots X_{12\cdots N}\Big],$$

where, in general,

$$I_{j(1)\cdots j(n)} = \prod_{i=1}^{n} \tilde{I}_{j(i)} B_{j(1)\cdots j(n)} \tag{34}$$

with

$$B_{j(1)\cdots j(n)} = \Big[1 + \sum_{p=1}^{n} \sum_{\langle l(1)\cdots l(p) | j(1)\cdots j(n)\rangle} \Big\{ \sum_{q=1}^{p} \sum_{\substack{\text{all partitions} \\ \text{of } l(1)\cdots l(p) \\ \text{among } p-q+1 \\ \text{factors}}} X_{\cdots} X_{\cdots} \cdots X_{\cdots} \Big\}\Big]. \tag{35}$$

To the right of 1 in each $B_{j(1)\cdots j(n)}$ there stands the sum of all normalized cluster integrals with indices comprising a subset of $\{j(1)\cdots j(n)\}$, plus the sum of all possible completely unlinked products of these normalized cluster integrals. A completely unlinked product is one in which no pair of factors has an index in common. More generally, an unlinked product of cluster integrals is one in which at least one factor has no index in common with any other factor. On the other hand if each factor has at least one index in common with one or more other factors, the product will be called linked.

Now, although termination of the series (35) for $B_{12\cdots N}$ at one-index, two-index, ... η-index, ... terms may lead to acceptable approximations for $B_{12\cdots N}$ when N is small, the non-uniform asymptotic N dependence of successive truncations indicates that, when N is large, some other form for $B_{12\cdots N}$ must be found for approximating $I(\alpha)$. This non-uniform N dependence results from the presence of the completely unlinked products.[13,17,22] Dropping terms which are of no consequence in the many-body limit (i.e. the limit in which $N \to \infty$ while ρ, the number density, is held constant), Iwamoto and Yamada[17] and Wu and Feenberg[24] have derived an expression for $B_{12\cdots N}$ in which all products of x's which appear are linked. Thus, upon writing

$$B_{12\cdots N} = \exp G_{IY} \tag{36}$$

they find in the many-body limit that

$$G_{IY} = \sum_{i=1}^{N} x_i + \sum_{i<j}^{N} x_{ij} + \sum_{i<j<k}^{N} [x_{ijk} - x_{ij}x_{jk} - x_{ij}x_{ik} - x_{ik}x_{jk}] + \cdots , \tag{37}$$

an expansion which, upon successive truncations, displays a uniform asymptotic N dependence. In the second paper of this series, we shall offer another method of rearranging $B_{12\cdots N}$ to generate such an exponential formula, a method which demonstrates, and utilizes, the (quite general) linked character of G_{IY}. Our procedure, unlike former ones, is applicable to finite as well as infinite systems.

By the order of a given term in (37) or in any cluster expansion based on the IY subnormalization integrals (29) we shall mean the number of distinct single-particle indices involved in any individual contribution to that term. This is a classification according to "number of bodies" - there will be one-body terms, two-body terms, three-body terms, ..., or, speaking more loosely, one-body clusters, two-body clusters, three-body clusters, ... - and is quite different from the ordering prescription of Clark and Westhaus[13] based on a "smallness parameter". In (37) the successive addends $\sum_i x_i$, $\sum_{i<j} x_{ij}$, $-\sum_{i<j<k} x_{ij}x_{jk}$, ... are, respectively, first-order, second-order, third-order, ... terms in the sense just defined.

In order to motivate the introduction of a well known alternative to the cluster formalism just discussed, let us suppose that a correlated wave function (12) with state-independent correlation

factors has been selected. Now consider a unitary transformation in the one-body vector space spanned by the set of single-particle functions $\varphi_1, \ldots, \varphi_N$:

$$\varphi_i(x) \longrightarrow \varphi_i'(x) = \sum_j U_{ij} \varphi_j(x), \quad i,j = 1, \ldots, N, \tag{38}$$

where

$$\sum_k U^*_{ki} U_{kj} = \sum_k U_{ik} U^*_{jk} = \delta_{ij} .$$

Since the replacement $\varphi_i \rightarrow \varphi_i'$, $i = 1, \ldots, N$, changes Φ by at most a phase factor, the expectation value $\langle S \rangle$ is invariant under this replacement. On the other hand, as one may readily verify, the IY expansion for $\langle S \rangle$ does not possess term by term nor indeed order by order invariance under the substitution (38). Of course, if summed to all orders, the expression $\prod_{i=1}^{N} \tilde{I}_i e^{G_{IY}}$ must yield $I_{(\alpha)}$ identically and thus lead to expectation values with the above invariance. But practical application of this cluster expansion theory demands that G_{IY} be terminated in low orders, whence the approximate expectation values lack a very desirable feature of the exact expectation value.[13,14]

A cluster expansion which is invariant term by term under such a unitary transformation of the orbitals has been investigated by Aviles[18] and by Hartogh and Tolhoek.[19] The quantities which are decomposed into cluster integrals are certain linear combinations,

or averages, of the subnormalization integrals defined in (29):

$$\begin{aligned}
\mathcal{I}_1 &= \frac{1}{N}\sum_{i=1}^{N} I_i \,, \\
\mathcal{I}_2 &= \frac{2}{N(N-1)}\sum_{i<j} I_{ij} \,, \\
&\vdots \\
\mathcal{I}_n &= \frac{n!\,(N-n)!}{N!}\sum_{\langle j(1)\cdots j(n)\rangle} I_{j(1)\cdots j(n)} \,, \\
&\vdots \\
\mathcal{I}_N &= I_{12\cdots N} = I(\alpha) \,.
\end{aligned} \tag{39}$$

These linear combinations are themselves invariant under the transformation (38) and so in turn will be the cluster integrals which they define. Having motivated the introduction of these new subnormalization integrals we may drop our restriction to the wave function (12). Upon so doing the above statements concerning invariance may no longer apply; we shall emphasize this fact by putting the word <u>invariant</u> within quotation marks from now on.

We proceed in analogy with the foregoing development, again first considering the situation in which no dynamical correlations exist among the particles and in which we need only be concerned with the one-body component of $S(1\cdots n)$. Here, in complete correspondence with (30), we have

$$\mathcal{L}_n \to \tilde{\mathcal{L}}_n = \frac{n!\,(N-n)!}{N!} \sum_{\langle j_{(1)} \cdots j_{(n)} \rangle}' \frac{1}{n!} \int \prod_{b=1}^{n} dx_b \begin{vmatrix} \varphi_{j_{(1)}}(x_1) & \cdots & \varphi_{j_{(n)}}(x_1) \\ \vdots & & \vdots \\ \varphi_{j_{(1)}}(x_n) & \cdots & \varphi_{j_{(n)}}(x_n) \end{vmatrix}^* e^{\alpha \sum_{i=1}^{n} \bar{S}_{1(i)}} \begin{vmatrix} \varphi_{j_{(1)}}(x_1) & \cdots & \varphi_{j_{(n)}}(x_1) \\ \vdots & & \vdots \\ \varphi_{j_{(1)}}(x_n) & \cdots & \varphi_{j_{(n)}}(x_n) \end{vmatrix}$$

$$= (\tilde{\mathcal{L}}_1)^n + O(\alpha^2), \tag{40}$$

where

$$\tilde{\mathcal{L}}_1 = \frac{1}{N} \sum_{i=1}^{N} \int dx_1 \varphi_i^*(x_1)\, e^{\alpha \bar{S}_{1(1)}}\, \varphi_i(x_1) = \frac{1}{N} \sum_{i=1}^{N} \tilde{I}_i \,. \tag{41}$$

Returning to the realistic situation, we "build up" $\mathcal{L}_n$ by replacing successive numbers of $\tilde{\mathcal{L}}_1$ factors in $(\tilde{\mathcal{L}}_1)^n$ with appropriate sums of products of cluster integrals. This process may be viewed alternatively as a decomposition of $\mathcal{L}_n$ into cluster integrals. From either point of view, of course, with $\tilde{\mathcal{L}}_1$, $\mathcal{L}_n$, and cluster integrals $\mathcal{K}_\rho$ $(\rho < n)$ having already been defined, it is the cluster integral $\mathcal{K}_n$ which is defined by this decomposition of $\mathcal{L}_n$. Beginning the process with $\mathcal{L}_1$, we write

$$\begin{aligned}
\mathcal{L}_1 &= \tilde{\mathcal{L}}_1 + \mathcal{K}_1 \,, \\
\mathcal{L}_2 &= \tilde{\mathcal{L}}_1^2 + 2\tilde{\mathcal{L}}_1 \mathcal{K}_1 + \mathcal{K}_1^2 + \mathcal{K}_2 \,, \\
\mathcal{L}_3 &= \tilde{\mathcal{L}}_1^3 + 3\tilde{\mathcal{L}}_1^2 \mathcal{K}_1 + 3\tilde{\mathcal{L}}_1 \mathcal{K}_1^2 + 3\tilde{\mathcal{L}}_1 \mathcal{K}_2 + \mathcal{K}_1^3 + 3\mathcal{K}_2 \mathcal{K}_1 + \mathcal{K}_3 \,, \\
&\vdots \\
\mathcal{L}_N &= \tilde{\mathcal{L}}_1^N + N\tilde{\mathcal{L}}_1^{N-1} \mathcal{K}_1 + \cdots \mathcal{K}_N \,.
\end{aligned} \tag{42}$$

Then, continuing the development in analogy with the decomposition of $I_{j(1),\ldots,j(n)}$, we define

$$x_n = \frac{\mathcal{X}_n}{(\tilde{\mathcal{L}}_1)^n} \tag{43}$$

and rewrite the general equation in the above set as

$$\mathcal{L}_n = (\tilde{\mathcal{L}}_1)^n B_n \tag{44}$$

with

$$B_n = \left\{1 + \sum_{p=1}^{n} p^{C_n} \sum_{\substack{\text{all partitions} \\ \text{such that} \\ \sum_{b=1}^{p} b\nu_b = p}} \frac{p!\, x_1^{\nu_1} \cdots x_b^{\nu_b} \cdots x_p^{\nu_p}}{\prod_{b=1}^{p} (b!)^{\nu_b} \nu_b!} \right\}. \tag{45}$$

Once more hoping to approximate B_N in terms of the few-body cluster integrals, say x_1, x_2, x_3, and x_4, we discover that in the case of large N the series (45) must first be rearranged in order to express B_N in terms of a series which, for large N, is uniform in N. And again the required rearrangement results in an exponential formula,

$$B_N = \exp g_{AHT}, \tag{46}$$

with g_{AHT} given, as the many-body limit is approached, by the "uniform" cluster expansion

$$g_{AHT} = N\chi_1 + \frac{N^2}{2!}\chi_2 + \frac{N^3}{3!}(\chi_3 - 3\chi_2^2) + \cdots \quad . \tag{47}$$

A derivation of (46), together with a generalization of (47) which includes those terms which must also be accounted for when N is not large, will be given in the second paper of this series, where the properties of the "factor-cluster" expansions introduced below are more fully exploited.

By the order of a given term in (47) or in any cluster expansion based on the AHT subnormalization integrals (39) we shall mean the following: in the case of the asymptotically leading terms, simply the power of N that appears explicitly; in the case of terms down from these by $O(1/N)$, the minimum number of sets of particle coordinates which must be introduced to carry out the integrations involved. This definition is not as arbitrary as it appears, since it will be seen to maintain a close correspondence with the "number-of-bodies" ordering prescription set up for expansions based on the IY subnormalization integrals. In (47) the successive addends $N\chi_1$, $\frac{1}{2}N^2\chi_2$, $-\frac{1}{2}N^3\chi_2^2$, ... are, respectively, first-order, second-order, third-order, ... terms in the sense just defined, while the asymptotically negligible term $\frac{1}{2}N\chi_1^2$, to be incorporated later, is of second order.

The necessity of rearranging the series for $B_{12\cdots N}$ and B_N has prompted us to seek new and "more natural" modes of decomposition to replace those of IY and AHT, modes which require no rearrangement to make sense for large N. The two alternative approaches

presented here are closely related to a cluster expansion proposed by Van Kampen[20] in the imperfect gas problem. They have the virtue of immediate applicability to finite as well as infinite many-body problems. The first, a "non-invariant" formalism, is based on the "non-invariant" subnormalization integrals of IY; the second, an "invariant" formalism, on the "invariant" subnormalization integrals of AHT.

Instead of constructing the $I_{j(1)\cdots j(n)}$ by replacing the $\tilde{I}_{j(i)}$'s in the product $\prod_{i=1}^{n} \tilde{I}_{j(i)}$ as we originally did in (31), we now propose that additional factors - the new cluster integrals - simply be attached to this product according to the following prescription:

$$
\begin{aligned}
I_{j(1)} &= \tilde{I}_{j(1)}\, Y_{j(1)} \,, \\
I_{j(1)j(2)} &= \tilde{I}_{j(1)}\, \tilde{I}_{j(2)}\, Y_{j(1)} \cdot Y_{j(2)} \cdot Y_{j(1)j(2)} \,, \\
I_{j(1)j(2)j(3)} &= \Big[\prod_{i=1}^{3} \tilde{I}_{j(i)}\Big] \cdot \Big[\prod_{l=1}^{3} Y_{j(l)}\Big] \cdot \Big[\prod_{1\le p<q\le 3} Y_{j(p)j(q)}\Big] \cdot Y_{j(1)j(2)j(3)} \,, \\
&\vdots \\
I_{12\cdots N} &= \Big[\prod_{i=1}^{N} \tilde{I}_{i}\Big] \cdot \Big[\prod_{l=1}^{N} Y_{l}\Big] \cdot \Big[\prod_{1\le p<q\le N} Y_{pq}\Big] \cdot \cdots Y_{12\cdots N} \,.
\end{aligned}
\tag{48}
$$

Employing (26) together with the final equation of this set, we arrive at an extremely simple formula for the expectation value

$$
\langle S \rangle = \sum_{i=1}^{N} \left. \frac{\frac{d}{d\alpha} \tilde{I}_i}{\tilde{I}_i} \right|_{\alpha=0} + \sum_{n=1}^{N} \sum_{\langle j(1)\cdots j(n)\rangle} \left. \frac{\frac{d}{d\alpha} Y_{j(1)\cdots j(n)}}{Y_{j(1)\cdots j(n)}} \right|_{\alpha=0} . \tag{49}
$$

Our general statements concerning cluster theories may be applied to this new mode of decomposing $I(\alpha)$. Specifically, the last cluster integral in (48) is defined in terms of the generalized normalization integral itself. But, of course, the hope is to approximate $\langle S \rangle$ by terminating the series in (49) after the first few sums, and thus avoid having to compute the many-indexed Y 's . The rapidity with which (49) converges depends ultimately upon the problem at hand; but that the series does depend uniformly on N in the many-body limit will become clear in the following paper where the relationship between this cluster expansion and that of IY is explored.

Implicit definitions of the quotients appearing in (49) may be obtained immediately upon differentiating the logarithm of each equation in the set (48) with respect to α . Defining

$$\tilde{J}_{j(i)} = \left. \frac{\frac{d}{d\alpha} \tilde{I}_{j(i)}}{\tilde{I}_{j(i)}} \right|_{\alpha=0}$$

$$J_{j(1)\cdots j(n)} = \left. \frac{\frac{d}{d\alpha} I_{j(1)\cdots j(n)}}{I_{j(1)\cdots j(n)}} \right|_{\alpha=0} \qquad (50)$$

and

$$Z_{j(1)\cdots j(n)} = \left. \frac{\frac{d}{d\alpha} Y_{j(1)\cdots j(n)}}{Y_{j(1)\cdots j(n)}} \right|_{\alpha=0} \qquad (51)$$

we have

$$J_{j(1)\cdots j(n)} = \sum_{i=1}^{n} \tilde{J}_{j(i)} + \sum_{q=1}^{n} \sum' \langle l(1)\cdots l(q) | j(1)\cdots j(n) \rangle Z_{l(1)\cdots l(q)} \qquad (52)$$

$$n = 1, \ldots, N.$$

The key to the inversion of this set of equations is the realization that the substitution for the $Z_{\ell(1)\cdots\ell(q)}$'s of their definitions in terms of the basic quantities $\tilde{J}_{\ell(i)}$ and $J_{\ell(1)\cdots\ell(p)}$ must transform these equations into identities. Hence we conclude that

$$Z_{j(i)} = J_{j(i)} - \tilde{J}_{j(i)} \,, \tag{53}$$

$$Z_{j(1)\cdots j(n)} = \sum_{q=1}^{n} (-1)^{n-q} \Big\{ \sum_{\langle \ell(1)\cdots\ell(q) | j(1)\cdots j(n)\rangle} J_{\ell(1)\cdots\ell(q)} \Big\} \,, \quad n \geq 2.$$

For upon the insertion of these relations into

$$J_{k(1)\cdots k(f)} = \sum_{i=1}^{f} \tilde{J}_{k(i)} + \sum_{p=1}^{f} \sum_{\langle h(1)\cdots h(p) | k(1)\cdots k(f)\rangle} Z_{h(1)\cdots h(p)}$$

the coefficient of each $\tilde{J}_{k(i)}$ vanishes, while the coefficient of $J_{\ell(1)\cdots\ell(q)}$ $\{\ell(1)\cdots\ell(q)\} \subset \{k(1)\cdots k(f)\}$, is given by

$$\sum_{s=q}^{f} (-1)^{s-q} \, {}_{s-q}C_{f-q} = \sum_{t=0}^{f-q} (-1)^{t} \, {}_{t}C_{f-q} = \begin{cases} 0 \,, & q < f \,, \\ 1 \,, & q = f \,, \end{cases}$$

as required. Note that the $\tilde{J}_{j(i)}$ enter only into the one-indexed cluster integrals. The results of this new "factor-cluster" formalism may be succintly stated as follows:

$$\langle S \rangle = \sum_{i=1}^{N} \tilde{J}_{i} + \sum_{n=1}^{N} \sum_{\langle j(1)\cdots j(n)\rangle} Z_{j(1)\cdots j(n)} \,, \tag{49}$$

where

$$Z_{j(i)} = J_{j(i)} - \tilde{J}_{j(i)} ,$$

$$Z_{j(1)\cdots j(n)} = \sum_{q=1}^{n} (-1)^{n-q} \Big\{ \sum_{\ell(1)\cdots\ell(q)\,|\,j(1)\cdots j(n)} J_{\ell(1)\cdots\ell(q)} \Big\}, \quad n \geq 2. \tag{53}$$

The quotients

$$\tilde{J}_{j(i)} = \frac{\frac{d}{d\alpha}\tilde{I}_{j(i)}}{\tilde{I}_{j(i)}}\Bigg|_{\alpha=0} = \frac{\int dx_1 \varphi^*_{j(i)}(x_1) \bar{S}_{1(1)} \varphi_{j(i)}(x_1)}{\int dx_1 \varphi^*_{j(i)}(x_1) \varphi_{j(i)}(x_1)}$$

and

$$J_{\ell(1)\cdots\ell(q)} = \frac{\frac{d}{d\alpha} I_{\ell(1)\cdots\ell(q)}}{I_{\ell(1)\cdots\ell(q)}}\Bigg|_{\alpha=0} = \frac{\int \prod_{b=1}^{q} dx_b \Psi^*_{\ell(1)\cdots\ell(q)} S_{(1\cdots q)} \Psi_{\ell(1)\cdots\ell(q)}}{\int \prod_{b=1}^{q} dx_b \Psi^*_{\ell(1)\cdots\ell(q)} \Psi_{\ell(1)\cdots\ell(q)}}$$

are not susceptible to further reductions and must therefore be evaluated as the basic ingredients of the expansion.

Let us now consider a factor decomposition alternative to (42). Again $\mathcal{L}_n$ is "built up" from $(\tilde{\mathcal{L}}_1)^n$ by attaching cluster integrals $\mathcal{Y}_p$ $(p \leq n)$ - and thus defining $\mathcal{Y}_n$ - in the following manner:

$$
\begin{aligned}
\mathcal{L}_1 &= \tilde{\mathcal{L}}_1 \cdot \mathcal{Y}_1 , \\
\mathcal{L}_2 &= \tilde{\mathcal{L}}_1^2 \cdot \mathcal{Y}_1^2 \cdot \mathcal{Y}_2 , \\
\mathcal{L}_3 &= \tilde{\mathcal{L}}_1^3 \cdot \mathcal{Y}_1^3 \cdot \mathcal{Y}_2^3 \, \mathcal{Y}_3 , \\
&\vdots \\
\mathcal{L}_n &= (\tilde{\mathcal{L}}_1)^n \cdot \Big[\prod_{k=1}^{n} (\mathcal{Y}_k)^{k C_n} \Big] , \\
&\vdots \\
\mathcal{L}_N &= \mathcal{I} = (\tilde{\mathcal{L}}_1)^N \cdot \Big[\prod_{k=1}^{N} (\mathcal{Y}_k)^{k C_N} \Big] .
\end{aligned}
\tag{54}
$$

Formulas completely analogous to (48) through (53) emerge. Indeed, we find that

$$
\mathcal{J}_n = n \tilde{\mathcal{J}}_1 + \sum_{k=1}^{n} k C_n \mathcal{J}_k \tag{55}
$$

and, in particular,

$$
\langle S \rangle = \mathcal{J}_N = N \tilde{\mathcal{J}}_1 + \sum_{k=1}^{N} k C_N \mathcal{J}_k , \tag{56}
$$

where we have defined

$$
\begin{aligned}
\tilde{\mathcal{J}}_1 &\equiv \left. \frac{\frac{d}{d\alpha} \tilde{\mathcal{L}}_1}{\tilde{\mathcal{L}}_1} \right|_{\alpha = 0} , \\
\mathcal{J}_n &\equiv \left. \frac{\frac{d}{d\alpha} \mathcal{L}_n}{\mathcal{L}_n} \right|_{\alpha = 0} ,
\end{aligned}
\tag{57}
$$

and

$$g_n \equiv \left. \frac{\frac{d}{d\alpha} y_n}{y_n} \right|_{\alpha=0} . \tag{58}$$

The inversion of (55) parallels that of (52). Here the required identity is ensured by taking

$$\begin{aligned} g_1 &= g_1 - \tilde{g}_1 \\ g_n &= \sum_{q=1}^{n} (-1)^{n-q} \frac{n!}{q!(n-q)!} g_q \qquad n \geq 2. \end{aligned} \tag{59}$$

Eq. (56) constitutes our newly-proposed "invariant"-factor-cluster expansion, with successive terms given by (59). The computation of the g_n must be carried out in terms of the basic ingredients, the "invariant" $\tilde{g}_1, g_n$'s of (57).

To keep the terminology and the various relationships straight, we list the four cluster formalims just analyzed:

1) the conventional one of IY, a "non-invariant" formalism in which a sum-of-factors decomposition law is postulated for the IY subnormalization integrals,

2) the conventional one of AHT, an "invariant" formalism in which a sum-of-factors decomposition law is postulated for the AHT subnormalization integrals,

3) a new "non-invariant-factor-cluster" formalism (henceforth,

the FIY formalism) in which a product decomposition law is postulated for the IY subnormalization integrals, and

4) a new "invariant-factor-cluster" formalism (henceforth, the FAHT formalism) in which a product decomposition law is postulated for the AHT subnormalization integrals.

There is one important feature of general cluster expansion theory that we have not explicitly pointed out: the arbitrariness of the n-body subnormalization integrals with $n<N$. Since, in any complete cluster expansion of $I(\alpha)$, the net coefficient of every subnormalization integral except the last one, $I_{1\ldots N} = I(\alpha) = \mathcal{I}_N$, is strictly zero, the subnormalization integrals with $n < N$ are entirely at our disposal. The choices (29), (39) are only two of an infinite number of possibilities. One should take advantage of this arbitrariness in tailoring the cluster formalism to the problem to be solved. An illuminating example of how this may be done is provided by the work of Feenberg and his collaborators on liquid He^3.[14,23]

3. An Application of the New "Invariant-Cluster" Formalism

We shall now apply the "invariant-factor-cluster" or FAHT formalism developed in the preceding section to the evaluation of the n-particle spatial distribution function (23). The resolution of the corresponding operator given in (24) leads to the following expressions for the basic invariants of the expansion:

$$\tilde{g}_1^{(n)}(r_1) = \begin{cases} \frac{1}{N}\sum_{i=1}^{N}\sum_{s_{z_1}}\sum_{t_{z_1}} \varphi_i^*(r_1, s_{z_1}, t_{z_1})\,\varphi_i(r_1, s_{z_1}, t_{z_1}), & n = 1, \\ 0, & n \geq 2, \end{cases} \tag{60}$$

$$g_q^{(n)}(r_1 \cdots r_n) = \begin{cases} \dfrac{\sum_{\langle \ell(1)\cdots\ell(q)\rangle} \frac{q!}{(q-n)!} \int \prod_{b=1}^{q} dx_b' \, \Psi^*_{\ell(1)\cdots\ell(q)}(x_1'\cdots x_q') \prod_{i=1}^{n} \delta(r_i - r_i')\, \Psi_{\ell(1)\cdots\ell(q)}(x_1'\cdots x_q')}{\sum_{\langle \ell(1)\cdots\ell(q)\rangle} \int \prod_{b=1}^{q} dx_b' \, \Psi^*_{\ell(1)\cdots\ell(q)}(x_1'\cdots x_q')\, \Psi_{\ell(1)\cdots\ell(q)}(x_1'\cdots x_q')}, & q \geq n, \\ 0, & q < n. \end{cases}$$

Thus, in accordance with formulas (56) - (59) the expansion for $\rho^{(n)}(r_1 \cdots r_n)$ takes the form

$$\rho^{(n)}(r_1 \cdots r_n) = N\tilde{g}_1^{(n)} + \sum_{k=1}^{N} {}^{k}C_N\, g_k^{(n)} \tag{61}$$

with

$$g_1^{(n)}(r_1) = \begin{cases} \frac{1}{N}\sum_{s_{z_1}}\sum_{t_{z_1}}\sum_{i=1}^{N}\left\{ \dfrac{\Psi_i^*(r_1, s_{z_1}, t_{z_1})\,\Psi_i(r_1, s_{z_1}, t_{z_1})}{\left[\sum_{j=1}^{N} \frac{1}{N}\int dx\, \Psi_j^*(x)\,\Psi_j(x)\right]} - \varphi_i^*(r_1, s_{z_1}, t_{z_1})\,\varphi_i(r_1, s_{z_1}, t_{z_1})\right\}, & n = 1, \\ 0, & n > 1, \end{cases} \tag{62}$$

$$g_q^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n) = \begin{cases} 0, & q < n, \\ \sum_{k=n}^{q} \frac{(-1)^{q-k} q!}{k!\,(q-k)!}\, g_k^{(n)} & \\ \quad \sum_{k=n}^{q} \frac{(-1)^{q-k}\, q!}{(q-k)!\,(k-n)!} \cdot \frac{\int \prod_{b=1}^{k} dx_b'\, D_k(x_1' \cdots x_k') \cdot \prod_{i=1}^{n} \delta(\underset{\sim}{r}_i - \underset{\sim}{r}_i')}{\int \prod_{b=1}^{k} dx_b'\, D_k(x_1' \cdots x_k')}, & q \geq n. \end{cases} \qquad (62 \text{ cont'd})$$

In arriving at the last line of (62) we have interchanged the integrations and summations which occur in both the numerator and denominator of the $g_k^{(n)}$'s and have defined

$$D_k(x_1' \cdots x_k') = \sum_{\langle \ell(1) \cdots \ell(k) \rangle} \Psi^*_{\ell(1) \cdots \ell(k)}(x_1' \cdots x_k')\, \Psi_{\ell(1) \cdots \ell(k)}(x_1' \cdots x_k') \,. \qquad (63)$$

Some intuitively satisfying features of this new cluster expansion deserve special study. First of all, since

$$\int d\underset{\sim}{r}_1 \cdots d\underset{\sim}{r}_n \left\{ \frac{\int \prod_{b=1}^{k} dx_b'\, D_k(x_1' \cdots x_k') \cdot \prod_{i=1}^{n} \delta(\underset{\sim}{r}_i - \underset{\sim}{r}_i')}{\int \prod_{b=1}^{k} dx_b'\, D_k(x_1' \cdots x_k')} \right\} = 1, \quad k \geq n, \qquad (64)$$

it follows that

$$\int d\underset{\sim}{r}_1\, \mathcal{J}_1^{(n)}(\underset{\sim}{r}_1) = 0, \quad \text{all } n; \quad \int d\underset{\sim}{r}_1\, \tilde{\mathcal{J}}_1^{(n)}(\underset{\sim}{r}_1) = \begin{cases} 1, & n=1, \\ 0, & n>1; \end{cases}$$

$$\int d\underset{\sim}{r}_1 \cdots d\underset{\sim}{r}_n\, \mathcal{J}_q^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n) \equiv 0, \quad q<n; \tag{65}$$

$$\int d\underset{\sim}{r}_1 \cdots d\underset{\sim}{r}_n\, \mathcal{J}_q^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n) = \sum_{k=n}^{q} \frac{(-1)^{q-k}\, q!}{(q-k)!\,(k-n)!} = \begin{cases} n!, & q=n,\ n>1, \\ 0, & q>n. \end{cases}$$

Thus the integral of the first non-vanishing term in the cluster expansion (61) provides the complete normalization, $N!/[(N-n)!]$, of $\rho^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n)$. There are no contributions to the normalization from higher orders. Moreover, to the extent that the ratio

$$\mathcal{R}_k(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n) = \frac{\int \prod_{b=1}^{k} dx'_b\, D_k(x'_1 \cdots x'_k) \prod_{i=1}^{n} \delta(\underset{\sim}{r}_i - \underset{\sim}{r}'_i)}{\int \prod_{b=1}^{k} dx'_b\, D_k(x'_1 \cdots x'_k)}, \quad k \geq n,$$

is independent of k, the quantities $\mathcal{J}_q^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n)$, $q>n$, vanish. For if we assume this ratio is independent of k and denote it by $\bar{\mathcal{R}}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n)$, we obtain directly from (62) that

$$\mathcal{J}_q^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n) = \bar{\mathcal{R}}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n) \cdot \sum_{k=n}^{q} \frac{(-1)^{q-k}\, q!}{(q-k)!\,(k-n)!} = \begin{cases} n!\, \bar{\mathcal{R}}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n), & q=n, \\ 0, & q>n. \end{cases} \tag{66}$$

Finally, employing two relations from combinatorial analysis, we are able to perform partial summations of the addends in (61)

resulting in a cogent expression for $\rho^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n)$ in terms of the fundamental "invariants", the $\mathcal{J}_p$'s . We need only recall that

$$\sum_{k=n}^{\mu} \sum_{q=n}^{k} F(q,k) = \sum_{q=n}^{\mu} \sum_{k=q}^{\mu} F(q,k) \tag{67}$$

and

$$\sum_{k=q}^{\mu} \frac{(-1)^{k-q}}{(N-k)!\,(k-q)!} = \sum_{j=0}^{\mu-q} \frac{(-1)^j (N-q)!}{(N-q-j)!\,j!} = \frac{(-1)^{\mu-q}(N-q-1)!}{(N-\mu-1)!\,(N-q)!} \tag{68}$$

in order to obtain for the sum of the first $\mu+1$ $(\mu \leq N)$ terms

$$N\mathcal{J}_1 + \sum_{k=1}^{\mu} {}_kC_N \mathcal{J}_k^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n) = N\tilde{\mathcal{J}}_1^{(n)} + \sum_{k=n}^{\mu} {}_kC_N \mathcal{J}_k^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n)$$

$$= \sum_{k=n}^{\mu} \sum_{q=n}^{k} \frac{N!}{k!(N-k)!} \cdot \frac{(-1)^{k-q} k!}{q!(k-q)!} \mathcal{J}_q^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n)$$

$$= \sum_{q=n}^{\mu} \left[\sum_{k=q}^{\mu} \frac{(-1)^{k-q} N!}{(N-k)!\,(k-q)!} \right] \frac{\mathcal{J}_q^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n)}{q!} \tag{69}$$

$$= \sum_{q=n}^{\mu} \left[\frac{(-1)^{\mu-q} N!\,(N-q-1)!}{(N-q)!\,(N-\mu-1)!\,(\mu-q)!} \cdot \frac{\mathcal{J}_q^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n)}{q!} \right].$$

This "invariant-factor-cluster" expansion of the n-particle spatial distribution function, unlike the corresponding AHT expansion generated via (46), (47), is applicable to finite as well as to infinite many-fermion systems. A reading of the following paper in this series will leave no doubt that, order by order, the terms by which the two expansions differ become negligible in the limit $N \longrightarrow \infty$. Hence, in treating infinitely extended fermion systems, the "invariant-factor-cluster" and the AHT formalisms yield the same spatial distribution functions order by order. However, this statement <u>cannot</u> be made about the spatial integral $\int d\underset{\sim}{r}_1 \cdots d\underset{\sim}{r}_n$ of the two expansions; the AHT expansion does not possess the desirable feature that only its first non-vanishing term contributes to the normalization of $\rho^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n)$.

It might be noted that relations analogous to (64) - (69) serve to establish completely analogous features of the FIY expansion for the n-particle spatial distribution function. And we might also note, explicitly, that the usual IY expansion for $\rho^{(n)}(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n)$ does not possess the very important feature of the FIY expansion that the only contribution to the normalization comes from the first non-vanishing term of the expansion.

The AHT expansion for the two-particle spatial distribution function has been studied in detail by Aviles[18] and by Hartogh and Tolhoek.[19] A numerical comparison of AHT and IY expansions for $\rho^{(2)}(\underset{\sim}{r}_1, \underset{\sim}{r}_2)$ was carried out by Woo in the framework of the liquid He^3 problem.[14]

We conclude this section with a study of $D_k(x_1 \cdots x_k)$ for the special case that Ψ is given by (12) - (14). Since the correlation function in the corresponding k-particle wave functions (cf. (27d)) is independent of orbital labels, the structure of $D_k(x_1 \cdots x_k)$ simplifies to

$$D_k(x_1 \cdots x_k) = \left[\prod_{j=1}^{k} \prod_{i} f_i^2(x_{\ell(i)} \cdots x_{\ell(j)})\right] \cdot \left\{\sum_{\langle q(1) \cdots q(k)\rangle} \Phi^*_{q(1)\cdots q(k)}(x_1 \cdots x_k)\Phi_{q(1)\cdots q(k)}(x_1 \cdots x_k)\right\} \cdot \tag{70}$$

Explicitly, the independent-particle-factor may be written

$$\Phi_{q(1)\cdots q(k)}(x_1 \cdots x_k) = \frac{1}{\sqrt{k!}} \det \Lambda_{q(1)\cdots q(k)}(x_1 \cdots x_k) \tag{71}$$

where

$$[\Lambda_{q(1)\cdots q(k)}]_{ij} = \varphi_{q(i)}(x_j) \quad , \quad i,j = 1, \cdots k \, . \tag{72}$$

Noting that

$$\Phi^*_{q(1)\cdots q(k)}(x_1 \cdots x_k)\Phi_{q(1)\cdots q(k)}(x_1 \cdots x_k) = \frac{1}{k!} \det \Lambda^*_{q(1)\cdots q(k)} \cdot \det \Lambda_{q(1)\cdots q(k)} \tag{73}$$

$$= \frac{1}{k!} \det\left[\Lambda^{\dagger}_{q(1)\cdots q(k)} \Lambda_{q(1)\cdots q(k)}\right],$$

Eq. (70) becomes

$$D_k(x_1 \cdots x_k) = \left[\prod_{j=1}^{k} \prod_{\langle \ell(1) \cdots \ell(j) | 1 \cdots k \rangle} f_j^2(x_{\ell(1)} \cdots \ell(j))\right] \cdot \left\{\frac{1}{k!} \sum_{\langle q(1) \cdots q(k) \rangle} \det Q_{q(1) \cdots q(k)}(x_1 \cdots x_k)\right\}, \tag{74}$$

the elements of the matrix

$$Q_{q(1) \cdots q(k)} = \Lambda^{+}_{q(1) \cdots q(k)} \Lambda_{q(1) \cdots q(k)} \tag{75}$$

being just

$$\left[Q_{q(1) \cdots q(k)}\right]_{ij} = \sum_{p=1}^{k} \varphi^{*}_{q(p)}(x_i) \varphi_{q(p)}(x_j) . \tag{76}$$

To carry the analysis further we must address ourselves to the crucial evaluation of the sum of determinants $\sum_{\langle q(1) \cdots q(k) \rangle} \det Q_{q(1) \cdots q(k)}$.

Each element of $Q_{q(1) \cdots q(k)}$ is the sum of the same k functions; the arguments of these functions vary from one element to another and thus serve as the row-column indices. Successive application of a well-known theorem governing the expansion of the determinant of a matrix in which each row of the i^{th} column is the sum of two terms allows us to express $\det Q_{q(1) \cdots q(k)}$ as the sum of k^k determinants:

$$\sum_{\langle q(1) \cdots q(k) \rangle} \det Q_{q(1) \cdots q(k)} = \sum_{\langle q(1) \cdots q(k) \rangle} \left\{ \sum_{j(1)=q(1)}^{q(k)} \cdots \sum_{j(k)=q(1)}^{q(k)} \begin{vmatrix} \varphi^{*}_{j(1)}(x_1) \varphi_{j(1)}(x_1) & \cdots & \varphi^{*}_{j(k)}(x_1) \varphi_{j(k)}(x_k) \\ \vdots & & \vdots \\ \varphi^{*}_{j(1)}(x_k) \varphi_{j(1)}(x_1) & \cdots & \varphi^{*}_{j(k)}(x_k) \varphi_{j(k)}(x_k) \end{vmatrix} \right\}. \tag{77}$$

Notice, however, that any term with $j(i) = j(\ell)$, $i \neq \ell$, is zero, for the determinant comprising that addend has two columns proportional. This observation may be repeated as we take into account the sum over the $N!/[(N-k)!\,k!]$ choices for the orbitals from among $\{\varphi_1, \cdots, \varphi_N\}$ with the result that

$$\sum_{\langle q(1)\cdots q(k)\rangle} \det Q_{q(1)\cdots q(k)} = \sum_{j(1)=1}^{N} \cdots \sum_{j(k)=1}^{N} \begin{vmatrix} \varphi^*_{j(1)}(x_1)\,\varphi_{j(1)}(x_1) & \cdots & \varphi^*_{j(k)}(x_1)\,\varphi_{j(k)}(x_k) \\ \vdots & & \vdots \\ \varphi^*_{j(1)}(x_k)\,\varphi_{j(1)}(x_1) & \cdots & \varphi^*_{j(k)}(x_k)\,\varphi_{j(k)}(x_k) \end{vmatrix} . \tag{78}$$

It now behooves us to reverse the procedure by which each $\det Q_{q(1)\cdots q(k)}$ was written as the sum of k^k determinants and thus express the right hand side of (78) as a single determinant. In this way we arrive at

$$\sum_{\langle q(1)\cdots q(k)\rangle} \det Q_{q(1)\cdots q(k)} = \begin{vmatrix} \sum_{i=1}^{N} \varphi^*_i(x_1)\,\varphi_i(x_1) & \cdots & \sum_{i=1}^{N} \varphi^*_i(x_1)\,\varphi_i(x_k) \\ \vdots & & \vdots \\ \sum_{i=1}^{N} \varphi^*_i(x_k)\,\varphi_i(x_1) & \cdots & \sum_{i=1}^{N} \varphi^*_i(x_k)\,\varphi_i(x_k) \end{vmatrix} \tag{79}$$

and thus, returning to (74), conclude that

$$D_k(x_1 \cdots x_k) = \left[\prod_{j=1}^{k} \prod_{\langle \ell_{(1)} \cdots \ell_{(j)} | 1 \cdots k \rangle} f_j^2(x_{\ell_{(1)}} \cdots x_{\ell_{(j)}}) \right] W_k(x_1 \cdots x_k) , \tag{80}$$

where

$$W_k(x_1 \cdots x_k) = \frac{1}{k!} \begin{vmatrix} \Delta(x_1,x_1) & \cdots & \Delta(x_1,x_k) \\ \vdots & & \vdots \\ \Delta(x_k,x_1) & \cdots & \Delta(x_k,x_k) \end{vmatrix} \tag{81}$$

and

$$\Delta(x_i,x_j) = \sum_{\ell=1}^{N} \varphi_\ell^*(x_i)\, \varphi_\ell(x_j) . \tag{82}$$

Thus the sum of products of determinants (70) has been reduced to a single determinant derived from a matrix whose elements, defined by (82), are easily shown to be invariant under the unitary transformation (38).

4. Comparison of the Four Cluster Formalisms

The factor-cluster formalisms - besides being directly useful for practical computation - provide a crutch for the extension of the IY and AHT formalisms to finite systems. In previous derivations, terms down from the leading terms in G_{IY} and G_{AHT} by $O(1/N)$ have

not been tracked down. These terms may now be generated as follows (we outline the procedure for the IY case): The final equations in (33) and (48) along with (34) and (36) imply that we must have, for all N ,

$$G_{IY} = \sum_{n=1}^{N} \sum_{\langle j(1)\cdots j(n)\rangle} \ln Y_{j(1)\cdots j(n)} \quad . \tag{83}$$

The equations which serve to decompose the $\ln I_{i(1)\cdots i(p)}$ in terms of the $\ln Y_{j(1)\cdots j(n)}, \{j(1)\cdots j(n)\} \subset \{i(1)\cdots i(p)\}$ are easily inverted (as usual one looks for an expression for $\ln Y_{j(1)\cdots j(n)}$ in terms of the $\ln I_{k(1)\cdots k(q)}, \{k(1)\cdots k(q)\} \subset \{j(1)\cdots j(n)\}$ which yields a set of identities). The $I_{k(1)\cdots k(q)}$ are then decomposed in the IY fashion in terms of the $I_{k(r)}, r = 1\cdots q$ and the $X_{l(1)\cdots l(s)}, \{l(1)\cdots l(s)\} \subset \{k(1)\cdots k(q)\}$. Upon expanding the logarithms there results for G_{IY} an expansion in the IY normalized cluster integrals which is valid for all N. Indeed, in this the IY case a linked cluster theorem may be proven: G_{IY} is the sum of all distinct $X_{\cdots}$'s and, with appropriate coefficients, all possible linked products of these cluster integrals. Corresponding to (83) we have, in the AHT case,

$$G_{AHT} = \sum_{n=1}^{N} {}_{n}C_{N} \ln Y_{n} \,, \tag{84}$$

and everything goes through in precisely the same way except that there is no question of a linked cluster theorem here since <u>linked product</u> is undefined in this formalism. It will be our task in the

following paper to carry out the program sketched in this paragraph; in particular we shall prove the linked cluster theorem for the IY expansion and contrive a rule for determining the aforementioned appropriate coefficients.

So, finally, one has four cluster expansions for $\langle S \rangle$, all valid for finite N as well as in the many-body limit. The "invariant" expansions (AHT and FAHT) clearly differ from the "non-invariant" expansions (IY and FIY) order by order as well as term by term. IY and FIY expansions, and on the other hand AHT and FAHT expansions, coincide order by order but not, of course, term by term.

The question naturally arises: Which is the best of these four formalisms to use in a given calculation? Assuredly, the answer to this question will depend on the details of the problem at hand. Nevertheless, some very general observations can be made, based on the fact that the IY (AHT) expansion for $\langle S \rangle$ may be derived from the FIY (FAHT) expansion by employing the procedure just described. As a result of the logarithmic expansions, there are, "in general" (i.e., there exist special exceptions as we shall see in a moment), an infinite number of non-negligible terms in each order of the IY and AHT expansions, even for finite N. On the other hand, the factorized expansions are characterized by a finite number of terms in each order, therefore a finite number of terms for finite N. (In fact there is just one term of each order in the FIY case as well as in the FAHT case if we obey our convention and regard each summand of $\sum_{n=1}^{N}$ as a single term.) Surely the only effect of the

extra expansions involved in the transition FIY → IY or FAHT → AHT is to lessen the rate of convergence of IY relative to FIY, AHT relative to FAHT. Clearly the order by order identity of IY and FIY (AHT and FAHT) expansions is of no practical significance if a given order in the IY (AHT) expansion contains an infinite number of terms.

For finite systems we may remove the qualification "in general" of the preceding paragraph. We expect a preference of FIY over IY, FAHT over AHT. But there is as yet no numerical evidence favoring one expansion over any of the others, even in a single particular case, since there has only been one cluster-method calculation on a finite system, that one using the IY procedure in the approximate evaluation of $\langle H \rangle$ for the O^{16} nucleus assuming a Jastrow trial wave function.[25,26]

Let us now consider extended systems with short range forces. We keep N finite but suppose it to be large enough that contributions $O(N^0)$ may be discarded compared with contributions $O(N)$. Then only a finite number of terms survive in a given order of the AHT expansion. Consequently the order by order identity of AHT and FAHT does, in this case, have practical significance. On the other hand the IY expansion does not necessarily so collapse. Let there exist for the observable S in question an irreducible resolution (18) - (19) such that, for some q, $S(1 \cdots q)$ is negligible for all configurations except those in which particles $j(1) \cdots j(p)$, $\{j(1) \cdots j(p)\} \subset \{1 \cdots q\}$, are within a volume

$O(\frac{1}{N})\Omega$, and is not identically zero. (The Hamiltonian H fits this requirement; the operator $P^{(n)}_{(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_n ; \underset{\sim}{r}_1' \cdots \underset{\sim}{r}_N')}$ whose expectation value yields the n-particle spatial distribution function does not.) If non-localized orbitals (with plane-wave spatial factors) are used, then all except a finite number of terms disappear from each order of the IY expansion. But if localized orbitals are used, there is no such simplification and there are still an infinite number of terms in each order. Proof of these statements rests upon the detailed results of the next paper; however, their plausibility may be enhanced at this point by a consideration of the following two terms - typical addends of the infinite sequences in question - contributing respectively to $\frac{\partial}{\partial \alpha} G_{IY}\Big|_{\alpha=0}$ and $\frac{\partial}{\partial \alpha} G_{AHT}\Big|_{\alpha=0}$:

$$\frac{\partial}{\partial \alpha} \sum_{i<j} x_{ij}^2 \Big|_{\alpha=0} ,$$

$$\frac{\partial}{\partial \alpha} \frac{N(N-1)}{2} x_{12}^2 \Big|_{\alpha=0} .$$

Thus in practical n-body cluster calculations of $\langle H \rangle$ for <u>extended systems</u> with short range forces it makes no difference whether we use the AHT or the FAHT expansion. For <u>quantum liquids</u> there will be no difference in practical IY and FIY calculations of this nature. For <u>quantum solids</u> there will be: indeed the numerical work of Nosanow and his collaborators[27] has revealed the expected superiority of the FIY formalism over the IY formalism in a variational

calculation of the cohesive energy of solid He^3 through three-body clusters assuming a Jastrow trial wave function.

There exists one last piece of information bearing on the comparison of the four formalisms in practical application. Through third order, IY and AHT results for the two-particle spatial distribution function in liquid He^3 assuming a Bose correlation factor are hardly distinguishable.[14,23]

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APPENDIX

The approximate evaluation of expectation values via the cluster expansion techniques of this paper may be carried through with any wave function once a method of defining the n-particle wave functions has been proposed. Among the possibilities considered in Section 1 is the exact N-particle wave function $\Psi_{\underset{\sim}{m}}$, written in the manner of Sinanoğlu:

$$\Psi_{\underset{\sim}{m}} = \mathcal{A}(N)\left[\prod_{i=1}^{N}\varphi_{m_i}(x_i) + \sum_{p}{}'\prod_{i\neq p}\varphi_{m_i}(x_i)\,U^{\underset{\sim}{m}}_{m_p}(x_p) + \right.$$
$$\left. \frac{1}{\sqrt{2!}}\sum_{p<q}{}'\prod_{i\neq p,q}\varphi_{m_i}(x_i)\,U^{\underset{\sim}{m}}_{m_p m_q}(x_p x_q) + \cdots \frac{1}{\sqrt{N!}}\,U^{\underset{\sim}{m}}_{m_1\cdots m_N}(x_1\cdots x_N)\right]. \tag{A1}$$

This appendix is devoted to an examination of Sinanoğlu's expression for $\Psi_{\underset{\sim}{m}}$ with the intention of illuminating its structure and that of the corresponding n-particle wave functions.

We note that in the language of a configuration interaction (CI) treatment

$$U^{\underset{\sim}{m}}_{m_{j(1)}\cdots m_{j(q)}}(x_1\cdots x_q) =$$
$$\sum_{x_1<\cdots<x_q;\,\underset{\sim}{x}\neq\underset{\sim}{m}} C_{m_N\cdots x_q\cdots x_1\cdots m_1;\,m_1\cdots m_N}\,\mathcal{A}(q)\left[\varphi_{x_1}(x_1)\cdots\varphi_{x_q}(x_q)\right] \tag{A2}$$

where in practice the coefficients must be determined by a perturbative or variational procedure but are formally given by

$$C_{m_N\cdots x_q\cdots x_1\cdots m_1;\,m_1\cdots m_{j(1)}\cdots m_{j(q)}\cdots m_N} = \tag{A3}$$
$$\int\prod_{b=1}^{N}dx'_b\left\{\mathcal{A}(N)\left[\varphi_{m_1}(x'_1)\cdots\varphi_{x_1}(x'_{j(1)})\cdots\varphi_{x_q}(x'_{j(q)})\cdots\varphi_{m_N}(x'_N)\right]\right\}^{*}\Psi_{\underset{\sim}{m}}(x'_1\cdots x'_N).$$

In (A2) the sum is over all combinations of q orbitals excluded from the set $\{m_1 \cdots m_N\}$. The expression for the correlation function $U^{\underset{\sim}{m}}_{m_{j(1)} \cdots m_{j(q)}}$ may be recast into a compact, but revealing, form. Upon inserting (A3) into (A2) and interchanging the sums and integrations which occur, we find that $U^{\underset{\sim}{m}}_{m_{j(1)} \cdots m_{j(q)}}$ may be written

$$U^{\underset{\sim}{m}}_{m_{j(1)} \cdots m_{j(q)}} = \tag{A4}$$

$$\frac{1}{\sqrt{N!\,q!}} \int \prod_{b=1}^{N} dx'_b \sum_{\substack{x_1 < \cdots < x_q \\ \notin \underset{\sim}{m}}} \begin{vmatrix} \varphi^*_{m_1}(x'_1) \cdots \varphi^*_{x_1}(x'_1) \cdots \varphi^*_{x_q}(x'_1) \cdots \varphi^*_{m_N}(x'_1) \\ \vdots \\ \varphi^*_{m_1}(x'_N) \cdots \varphi^*_{x_1}(x'_N) \cdots \varphi^*_{x_q}(x'_N) \cdots \varphi^*_{m_N}(x'_N) \end{vmatrix} \cdot \begin{vmatrix} 1 & 0 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ 0 & 1 & & \vdots & & \vdots & & \\ \vdots & & \ddots & \varphi_{x_1}(x_1) & \cdots & \varphi_{x_q}(x_1) & & \\ & & & \vdots & & \vdots & & \\ 0 & & & \varphi_{x_1}(x_q) & \cdots & \varphi_{x_q}(x_q) & & \\ \vdots & & & \vdots & & \vdots & \ddots & 0 \\ 0 & \cdots & & 0 & & 0 & & 1 \end{vmatrix}$$

$$\times \bar{\Psi}_{\underset{\sim}{m}}(x'_1 \cdots x'_N)$$

The integrand may be simplified according to the following scheme: For a given set of q orbital labels $x_1 \cdots x_q$ the product of two determinants found in (A4) can be written as a single determinant,

$$\det \Theta^{x_1 \cdots x_q}_{m_{j(1)} \cdots m_{j(q)}} =$$

$$\begin{vmatrix} \varphi^*_{m_1}(x'_1) & \cdots & \sum_{i=1}^{q} \varphi^*_{x_i}(x'_1)\varphi_{x_i}(x_1) & \cdots & \sum_{i=1}^{q} \varphi^*_{x_i}(x'_1)\varphi_{x_i}(x_q) & \cdots & \varphi^*_{m_N}(x'_1) \\ \vdots & & \vdots & & \vdots & & \vdots \\ \varphi^*_{m_1}(x'_N) & \cdots & \sum_{i=1}^{q} \varphi^*_{x_i}(x'_N)\varphi_{x_i}(x_1) & \cdots & \sum_{i=1}^{q} \varphi^*_{x_i}(x'_N)\varphi_{x_i}(x_q) & \cdots & \varphi^*_{m_N}(x'_N) \end{vmatrix},$$

that is, a determinant in which the s^{th} row of the t^{th} column - occupied in $\Phi_{\underset{\sim}{m}}(x_1' \cdots x_N')$ by $\varphi_{m_t}(x_s)$ - is now given by

$$\left[\Theta^{x_1 \cdots x_q}_{m_{j(1)} \cdots m_{j(q)}}\right]_{st} = \begin{cases} \sum_{i=1}^{2} \varphi^*_{x_i}(x_s')\,\varphi_{x_i}(x_\ell), & \text{if } t = j(\ell),\ j(\ell) \in \{j(1) \cdots j(q)\} \\ \varphi^*_{m_t}(x_s') & \text{if } t \notin \{j(1) \cdots j(q)\} \end{cases} \tag{A5}$$

Moreover, by a procedure like that which leads from (73) to (79), the sum of such determinants may be reduced to a single determinant so that

$$\sum_{x_1 < \cdots < x_q \notin \underset{\sim}{m}} \det \Theta^{x_1 \cdots x_q}_{m_{j(1)} \cdots m_{j(q)}} =$$

$$\begin{vmatrix} \varphi^*_{m_1}(x_1') & \cdots & \sum_{x \notin \underset{\sim}{m}} \varphi^*_x(x_1')\,\varphi_x(x_1) & \cdots & \sum_{x \notin \underset{\sim}{m}} \varphi^*_x(x_1')\,\varphi_x(x_q) & \cdots & \varphi^*_{m_N}(x_1') \\ \vdots & & & & & & \\ \varphi^*_{m_1}(x_N') & \cdots & \sum_{x \notin \underset{\sim}{m}} \varphi^*_x(x_N')\,\varphi_x(x_1) & \cdots & \sum_{x \notin \underset{\sim}{m}} \varphi^*_x(x_N')\,\varphi_x(x_q) & \cdots & \varphi^*_{m_N}(x_N') \end{vmatrix} . \tag{A6}$$

Each of the sums appearing in (A6) is over all orbital labels $\alpha \notin \{m_1 \cdots m_N\}$. Since the single-particle states form an orthonormal basis in the one-particle Hilbert space, we can write

$$\sum_{\alpha \notin \underset{\sim}{m}}{}' \varphi^*_\alpha(x') \varphi_\alpha(x) = \delta(x', x) - \sum_{i=1}^{N} \varphi^*_{m_i}(x') \varphi_{m_i}(x) . \tag{A7}$$

Upon substituting this expression into (A6) we discover that, in addition to $\delta(x', x)$, only the terms involving $\varphi^*_{m_\ell}(x') \varphi_{m_\ell}(x)$ with $\ell \in \{j(1) \cdots j(q)\}$ give rise to non-vanishing contributions when the resulting determinant is expanded. Thus, we define

$$\mathcal{D}_{m_{j(1)} \cdots m_{j(q)}}(x_s, x_t) = \delta(x_s, x_t) - \sum_{i=1}^{q} \varphi^*_{m_{j(i)}}(x_s) \varphi_{m_{j(i)}}(x_t) \tag{A8}$$

and arrive at the result

$$U^{\underset{\sim}{m}}_{m_{j(1)} \cdots m_{j(q)}}(x_1 \cdots x_q) =$$

$$\frac{1}{\sqrt{N!\,q!}} \int \prod_{b=1}^{N} dx'_b \begin{vmatrix} \varphi^*_{m_1}(x'_1) & \cdots & \mathcal{D}_{m_{j(1)} \cdots m_{j(q)}}(x'_1, x_1) & \cdots & \mathcal{D}_{m_{j(1)} \cdots m_{j(q)}}(x'_1, x_q) & \cdots & \varphi^*_{m_N}(x'_1) \\ \vdots & & \vdots & & \vdots & & \vdots \\ \varphi^*_{m_1}(x'_N) & \cdots & \mathcal{D}_{m_{j(1)} \cdots m_{j(q)}}(x'_N, x_1) & \cdots & \mathcal{D}_{m_{j(1)} \cdots m_{j(q)}}(x'_N, x_q) & \cdots & \varphi^*_{m_N}(x'_N) \end{vmatrix} \Psi_{\underset{\sim}{m}}(x'_1 \cdots x'_N)$$

$$= \sqrt{\frac{N!}{q!}} \int \prod_{b=1}^{N} dx'_b \left\{ \varphi^*_{m_1}(x'_1) \cdots \mathcal{D}_{m_{j(1)} \cdots m_{j(q)}}(x'_{j(1)}, x_1) \cdots \mathcal{D}_{m_{j(1)} \cdots m_{j(q)}}(x'_{j(q)}, x_q) \cdots \varphi^*_{m_N}(x'_N) \right\} \Psi_{\underset{\sim}{m}}(x'_1 \cdots x'_N) .$$

(A9)

The second expression, in which the determinant has been replaced by a simple product, is obtained by recognizing that $\bar{\Psi}_{\hat{m}}(x_1' \cdots x_N')$ must be antisymmetric under the interchange of any two particle labels.

Although we have assumed $\Psi_{\underset{\sim}{m}}(x_1' \cdots x_N')$ to be the exact N particle wave function, the above derivation of (A9) may be bypassed and this formula viewed as a starting point for the analysis of trial wave functions.[5] Thus given a trial wave function $\tilde{\Psi}_{\underset{\sim}{m}}(x_1' \cdots x_N')$ (which may or may not turn out to be the sought-for eigenfunction) the corresponding correlation functions $\tilde{U}^{\underset{\sim}{m}}_{m_{j(1)} \cdots m_{j(q)}}$ from which to construct the "η-particle wave functions" may be found via (A9). If, as in accordance with (27b), we define

$$\tilde{\Psi}_{m_{j(1)} \cdots m_{j(n)}}(x_1 \cdots x_n) = \sqrt{\frac{n!}{N!}}\, Q(n) \Big[\prod_{i=1}^{n} \varphi_{m_{j(i)}}(x_i) + \sum_{p} \prod_{i=1,\, i \neq p}^{n} \varphi_{m_{j(i)}}(x_i)\, \tilde{U}^{\underset{\sim}{m}}_{m_{j(p)}}(x_p)$$
$$+ \frac{1}{\sqrt{2!}} \sum_{p<q} \prod_{i \neq p,q}^{n} \varphi_{m_{j(i)}}(x_i)\, \tilde{U}^{\underset{\sim}{m}}_{m_{j(p)} m_{j(q)}}(x_p, x_q) + \cdots \frac{1}{\sqrt{n!}}\, \tilde{U}^{\underset{\sim}{m}}_{m_{j(1)} \cdots m_{j(n)}}(x_1 \cdots x_n) \Big],$$

then the insertion of A(9) for the $\tilde{U}^{\underset{\sim}{m}}_{m_{\ell(1)} \cdots m_{\ell(p)}}$ yields the very natural expression

$$\tilde{\Psi}_{m_{j(1)} \cdots m_{j(n)}}(x_1 \cdots x_n) = \int \prod_{b=1}^{N} dx_b' \Big[\prod_{i=1}^{n} \delta(x_{j(i)}' - x_i) \prod_{p=1,\, p \notin \{j(1) \cdots j(n)\}}^{N} \varphi^*_{m_p}(x_p') \Big] \tilde{\Psi}_{\underset{\sim}{m}}(x_1' \cdots x_N').$$

(A10)

We have developed an explicit means of constructing the n-particle wave function from a given form for $\Psi_{\underset{\sim}{m}}(x_1 \cdots x_N)$. Certainly our prescription is not unique. Indeed, since completely summing any cluster expansion for $\langle S \rangle$ leaves a final expression involving only the N-body wave function $\Psi_{\underset{\sim}{m}}(x_1 \cdots x_N)$, we must admit that from a formal standpoint $\Psi_{m_{j(1)} \cdots m_{j(n)}}$ (with $n < N$) may be defined quite arbitrarily. Nevertheless, we anticipate that the method outlined here, resulting in the intuitively natural form for $\Psi_{m_{j(1)} \cdots m_{j(n)}}$ as evidenced in (A10), will prove most advantageous. Moreover, when the problem at hand allows the particles to be divided into subgroups such that the members of one subgroup are only weakly correlated with those of another, $\Psi_{m_{j(1)} \cdots m_{j(n)}}(x_1 \cdots x_n)$ as defined by (A10) approximates the probability amplitude[28] for such a subgroup of n particles, these particles occupying orbitals $\varphi_{m_{j(1)}} \cdots \varphi_{m_{j(n)}}$ in the independent-particle picture. Finally, we observe that the n-particle wave functions defined in (27c) and (27d) are not equivalent to the function (A10) but involve the further step of replacing some of the correlation functions within the integrand of (A10) by unity.

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